Boundary susceptibility in the open XXZ-chain

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Abstract. In the first part we calculate the boundary susceptibility χ_B in the open XXZ-chain at zero temperature and arbitrary magnetic field h by Bethe ansatz. We present analytical results for the leading terms when $|h| \ll \alpha$, where α is a known scale, and a numerical solution for the entire range of fields. In the second part we calculate susceptibility profiles near the boundary at finite temperature T numerically by using the density-matrix renormalization group for transfer matrices and analytically for $T \ll 1$ by field theoretical methods. Finally we compare χ_B at finite temperature with a low-temperature asymptotics which we obtain by combining our Bethe ansatz result with recent predictions from bosonization.

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1. Introduction

Even a single impurity can have a drastic effect on the low-energy properties of a one-dimensional interacting electron system. One of the simplest examples is an antiferromagnetic spin-1/2 chain with a non-magnetic impurity which cuts the chain and leads to a system with essentially free boundaries. Because translational invariance is broken the one-point correlation function $\langle S^z(r)\rangle$ is no longer independent from the site index r and the local susceptibility $\chi(r)$ acquires a nonzero alternating part [1]. Furthermore, the asymptotic behavior of correlation functions near such a boundary is no longer governed by the bulk critical exponents but instead by so called boundary or surface critical exponents [2, 3]. It is interesting to consider the case when the spin chain is not cut but instead one of the links is only slightly weaker.

$$\begin{aligned} H = J \sum_{r=1}^{N-1} \left(S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta S_r^z S_{r+1}^z \right) \\ + J_1' \left(S_1^x S_N^x + S_1^y S_N^y \right) + J_2' \Delta S_1^z S_N^z \end{aligned} \tag{1}$$

Here $J > 0$, $J_{1,2}' > 0$ and we have allowed for an XXZ-type anisotropy which is described by the parameter

$$\Delta =: \cos\gamma \text{ with } 0 \le \Delta \le 1 \;\; (0 \le \gamma \le \pi/2)\,. \tag{2}$$

Using the Jordan-Wigner transformation one can also think about this system as a lattice model of spinless Fermions with a repulsive density-density interaction

$$H = \frac{J}{2}\sum_{r=1}^{N-1}\left(c_r^\dagger c_{r+1} + h.c.\right) + \Delta J \sum_{r=1}^{N-1}\left(n_r - \frac{1}{2}\right)\left(n_{r+1} - \frac{1}{2}\right) + \frac{J_1'}{2}\left(c_1^\dagger c_N + h.c.\right) + \Delta J_2'\left(n_1 - \frac{1}{2}\right)\left(n_N - \frac{1}{2}\right) . \quad (3)$$

Therefore $J_1' = J - \delta J$ with $0 < \delta J \ll J$ corresponds to a weakening of the hopping amplitude whereas $J_2' = J - \delta J$ gives a weakened density-density interaction along one bond. For all Δ both perturbations have the same scaling dimension $x = K/2$ where $K = \pi/(\pi - \gamma)$ is the Luttinger parameter [4]. Weakening the hopping or the interaction along one bond is therefore always relevant‡. Assuming that the open chain presents the only stable fixed point one therefore expects that the physics at energies below $T_K/J \sim (\delta J/J)^{1/x}$ is governed by the open XXZ-chain [5]. This is the motivation to consider in the following only the open boundary condition (OBC) $J_1' = J_2' = 0$.

In an open XXZ-chain the free boundaries induce corrections of order $1/N$ to the bulk limit§. In particular a $1/N$-term in the susceptibility is expected which we denote hereafter as *boundary susceptibility* $\chi_B(h, T)$. From the scaling arguments given before it follows that a long chain with a finite concentration of impurities is effectively cut into pieces of finite length. Measurements of the susceptibility on such a system will therefore reveal large contributions from the boundaries. This has inspired a lot of theoretical work to actually calculate these boundary corrections [7, 8, 9, 10, 11, 12]. Very recently the leading contributions to the boundary susceptibility for $h \ll 1$ and $T \ll 1$ have been calculated by field theoretical methods [11, 12]. On the other hand it is also known that the XXZ-chain with OBC is exactly solvable by Bethe ansatz (BA) [13, 14]. For zero temperature, however, only the leading functional dependence on h for the isotropic case $\chi_B(h, T = 0) \sim 1/h(\ln h)^2$ has been calculated so far [9, 10, 15]. For finite temperatures de Sa and Tsvelik [7] have applied the thermodynamic Bethe Ansatz (TBA) in the anisotropic case. Evaluating their TBA equations and comparing with a numerical solution (see section 4) we have found that their results are wrong for all anisotropies. Even the free Fermion case (see section 2) is not reproduced correctly and there is also disagreement with the field theoretical results by Fujimoto and Eggert [11] and Furusaki and Hikihara [12] at low temperatures. Frahm and Zvyagin [15] have treated the isotropic case with the same TBA technique. Although at least the functional form for low temperatures is correct, their results are not reliable for high temperatures [16]. This raises the question if the TBA is applicable at all for OBC or at least which modifications have to be incorporated compared to the well known case of periodic boundary conditions (PBC).

Our paper is organized as follows: We start with the simple but instructive free Fermion case and establish results for the boundary susceptibility both as a function of T and h in section 2. In section 3 we report the Bethe ansatz solution for $T = 0$ and anisotropy $0 \le \Delta \le 1$. We present analytical results for the boundary susceptibility at $|h| \ll 1$ and a numerical solution of the BA formulas for arbitrary h. In section 4 we calculate susceptibility profiles near the boundary numerically by the density-matrix

‡ For the free Fermion case $K = 2$ the perturbation becomes marginal.

§ Note that in the periodic case no $1/N$ corrections exists and the first correction to the bulk limit is of order $1/N^2$ and determines the central charge [6].

renormalization group for transfer matrices (TMRG) and analytically by field theory methods. We also compare our numerical results for $\chi_B(h=0,T)$ with an analytical formula for $T \ll 1$ which we obtain by combining our BA results from section 3 with recent results from bosonization [11, 12]. The last section presents a summary and conclusions.

2. Free spinless Fermions

Here we want to consider the special case $\Delta = 0$ where eq. (3) describes noninteracting spinless Fermions. After Fourier transform the Hamiltonian takes the form

$$H = \sum_{n=1}^{N} (J\cos k_n + h)\left(c^\dagger_{k_n} c_{k_n} + h.c.\right) \quad \text{with} \quad k_n = \frac{\pi}{N+1} n \tag{4}$$

where we have included a magnetic field h. Note that the only difference to PBC are the momenta k_n which in this case would be given by $k_n = 2\pi/N$. The susceptibility is easily obtained as

$$\chi(h,T) = \frac{1}{4T}\sum_n \cosh^{-2}\left[\frac{1}{2T}(J\cos k_n + h)\right] \tag{5}$$

and using the Euler-MacLaurin formula then yields

$$\begin{aligned}
\chi(h,T) \quad &= \chi_{\text{bulk}}(h,T) + \frac{1}{N}\chi_B(h,T) + \mathrm{O}\left(\frac{1}{N^2}\right) \quad \text{with} \\
\chi_{\text{bulk}}(h,T) &= \frac{1}{4\pi T}\int_0^\pi \cosh^{-2}\left[\frac{1}{2T}(J\cos k + h)\right] dk \\
\chi_B(h,T) \quad &= \frac{1}{4\pi T}\int_0^\pi \cosh^{-2}\left[\frac{1}{2T}(J\cos k + h)\right] dk \\
&- \frac{1}{8T}\cosh^{-2}\left[\frac{1}{2T}(J+h)\right] - \frac{1}{8T}\cosh^{-2}\left[\frac{1}{2T}(J-h)\right] .
\end{aligned} \tag{6}$$

Therefore bulk and boundary susceptibility are identical at $T = 0$ and given by

$$\chi_{\text{bulk}}(h, T=0) = \chi_B(h, T=0) = \frac{1}{J\pi}\frac{1}{\sqrt{1-(h/J)^2}} . \tag{7}$$

At finite temperatures χ_{bulk} and χ_B are different, however, the additional factors in χ_B vanish exponentially for $T \to 0$ so that they still share the same low-temperature asymptotics

$$\chi_{\text{bulk}}(h=0, T\to 0) = \chi_B(h=0, T\to 0) = \frac{1}{J\pi} + \frac{\pi}{6J^3}T^2 + \mathrm{O}\left(T^4\right) . \tag{8}$$

Fig. 1 shows the boundary and bulk susceptibilities for finite temperature at $h = 0$ and as a function of h at $T = 0$ (inset). In the next section we will discuss the BA solution for $T = 0$. We will see that a finite interaction between the Fermions, $\Delta \neq 0$, has dramatic effects and $\chi_{\text{bulk}}(h, T = 0)$ and $\chi_B(h, T = 0)$ are no longer identical. For $1/2 \leq \Delta \leq 1$ we find that $\chi_B(h, T = 0)$ even diverges for $h \to 0$ whereas $\chi_{\text{bulk}}(h = 0, T = 0)$ remains always finite.

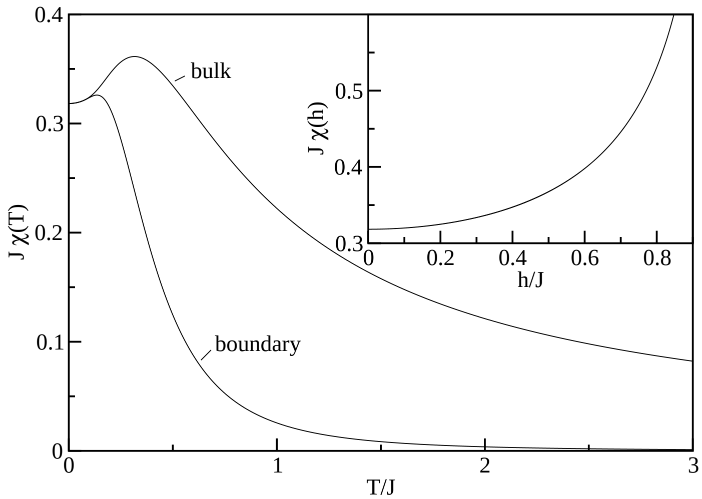

Figure 1. Bulk and boundary susceptibilities for free Fermions. Note that $\chi(h, T = 0)$ diverges for $h \to h_c = J$.

3. The Bethe ansatz solution

In this section we calculate ground-state properties of the model (1), i.e. $T = 0$. The Hamiltonian (1) with $J_1' = J_2' = 0$ has been diagonalized both by coordinate and algebraic Bethe Ansatz [13, 14]. In the following, we refer to the algebraic Bethe Ansatz [14]. The eigenvalues E are parameterized by a set of M-many quantum numbers $\{\lambda_1, \ldots, \lambda_M\}$,

$$E = J\left[-\sum_{j=1}^{M} \frac{\sin^2\gamma}{\cosh(2\lambda_j) - \cos\gamma} + \frac{N-1}{4}\cos\gamma\right] - hS^z \tag{9}$$

$$S^z = N/2 - M. \tag{10}$$

Here, S^z is the total z-component of the spin, h a magnetic field along the z-direction and we always assume in the following $h \geq 0$ without loss of generality. The anisotropic exchange constant Δ is given by eq. (2) and the λ_k are determined by the following set of coupled algebraic equations

$$\frac{\phi(\lambda_k + \mathrm{i}\gamma/2)}{\phi(\lambda_k - \mathrm{i}\gamma/2)} \frac{a(2\lambda_k, \gamma)a(\lambda_k, \pi/2 - \gamma/2)a(\lambda_k, \pi/2 - \gamma/2)}{a(2\lambda_k, -\gamma)a(\lambda_k, -\pi/2 + \gamma/2)a(\lambda_k, -\pi/2 + \gamma/2)} = -\frac{q_M(\lambda_k + \mathrm{i}\gamma)q_M(-\lambda_k - \mathrm{i}\gamma)}{q_M(\lambda_k - \mathrm{i}\gamma)q_M(-\lambda_k + \mathrm{i}\gamma)}, \tag{11}$$

with the definitions

$$\phi(\lambda) := \sinh^{2N}(\lambda) \quad , \quad a(\lambda, \mu) := \sinh(\lambda + \mathrm{i}\mu) \quad , \quad q_M(\lambda) := \prod_{j=1}^{M} \sinh(\lambda - \lambda_j) \, .$$

We first deal with the anisotropic case $0 < \gamma \leq \pi/2$ and obtain equations for the susceptibility, which are solved analytically in the limit of small magnetic field. The isotropic case is treated afterwards. At the end of this section, we present numerical results for the susceptibility at arbitrary magnetic field.

3.1. Anisotropic case

The solutions to (11) are periodic in the complex plane with period $2\pi\mathrm{i}$, so that we can focus on a strip parallel to the real axis with width $2\pi\mathrm{i}$. Using arguments of analyticity, one sees that there are $2N+3+2M$ roots in such a strip. So besides the M-many λ_k which yield the energy eigenvalues (9), there are $2N+3+M$ additional roots. Consider now the strip with Im $\lambda_k \in]-\pi,\pi]\,\forall k$. We denote the roots in this set by $\{\lambda_1,\ldots,\lambda_M,\lambda_1^{(h)},\ldots,\lambda_{2N+M}^{(h)},0,-\mathrm{i}\pi/2,\mathrm{i}\pi/2\}$. It is straightforward to verify that $0,\pm\mathrm{i}\pi/2$ are roots. However, the algebraic Bethe Ansatz fails for these roots so that these solutions must be excluded. The roots are distributed symmetrically, both with respect to the real and imaginary axis. In this work we focus on the calculation of the ground state energy where $M=N/2$ and $\lambda_j \in \mathbb{R}^{>0}\,\forall j$. Then there are $N/2$ roots $\lambda_j^{(h)} = -\lambda_j$, $j=1,\ldots,N/2$. A numerical evaluation of (11) shows that the remaining roots $\lambda^{(h)}_{j=N/2+1,\ldots 3N/2}$ ($\lambda^{(h)}_{j=3N/2+1,\ldots 5N/2}$) have imaginary part $-\mathrm{i}\gamma/2$ ($\mathrm{i}\gamma/2$). The eigenvalues E are symmetrical in the λ_j. We thus want to deal with the set $\{v_1,\ldots,v_N\} := \{\lambda^{(h)}_{N/2},\ldots,\lambda_1^{(h)},\lambda_1,\ldots,\lambda_{N/2}\}$, whose elements are distributed symmetrically on the real axis w.r.t. the origin. From (11), we find that the v_j are the N real solutions to the equations

$$\frac{\phi(v_m+\mathrm{i}\gamma/2)}{\phi(v_m-\mathrm{i}\gamma/2)}\left[\frac{a(v_m,\pi/2-\gamma/2)\,a(v_m,\gamma/2)}{a(v_m,-\pi/2+\gamma/2)\,a(v_m,-\gamma/2)}\right] = \frac{q_N(v_m+\mathrm{i}\gamma)}{q_N(v_m-\mathrm{i}\gamma)}. \tag{12}$$

The remaining $2N$ solutions $v_j^{(h)}$ are identified as $v^{(h)}_{j=1,\ldots,2N} \equiv \lambda^{(h)}_{j=N/2+1,\ldots,5N/2}$. In (12), the terms in brackets $[\cdots]$ are due to the OBC. These terms would be absent in the case of PBC.

Our aim is to calculate the $1/N$-contribution to the ground state energy per lattice site in the thermodynamical limit (TL). Like in the PBC-case [17, 18], we introduce the density of roots on the real axis,

$$\begin{aligned}\Delta_{v_m} \quad &:= \frac{v_m+v_{m+1}}{2} - \frac{v_{m-1}+v_m}{2}\,, \qquad m=2,\ldots,N-1\\ \rho_+(v_m) &:= \frac{1}{2N\,\Delta_{v_m}},\end{aligned} \tag{13}$$

where Δ_{v_m} is the distance between two points on the left and on the right of the root v_m, such that the left (right) point is situated midway between v_{m-1},v_m (v_m,v_{m+1}). From numerical studies the boundary values of ρ_+ are inferred, $\rho_+(v_1)=\rho_+(v_N)=0$, with $\rho_+(v_{1,N})\Delta_{v_{1,N}}=1$. Together with (13) it follows that

$$\sum_{m=1}^{N} \rho_+(v_m)\Delta_{v_m} = \frac{1}{2}\,. \tag{14}$$

In the TL $\Delta_{v_m}\to 0$ and $\rho_+(v_m)$ becomes a smooth function. Let us define the interval with non-vanishing density by $[-B,B]$, i.e. $v_1\to -B$, $v_N\to B$ in the TL. Then sums over functions $f(v_k)$ are transformed into integrals by

$$\sum_{k=1}^{N}\frac{1}{2N}f(v_k) = \int_{-B}^{B} f(x)\rho_+(x)\mathrm{d}x - \frac{1}{2N}f(0) + \mathrm{O}(1/N^2),$$

where the contribution $f(0)$ is subtracted because the algebraic Bethe Ansatz fails at the origin. There are no further $\mathrm{O}(1/N)$-terms because ρ_+ vanishes outside the integration boundaries by definition,

$$\rho_+(v) \equiv \rho_+(v)\theta(-v+B)\theta(B+v)\,,$$

where $\theta(v)$ is the Heaviside-function. In order to find the continuum version of (12), it is convenient to define

$$\rho(v) := \rho_+(v) + \rho_-(v)$$
$$\rho_-(v) := \rho(v)(\theta(v-B) + \theta(-B-v))\,.$$

By taking the logarithmic derivative, the continuum version of (12) is obtained

$$\vartheta(x,\gamma) + \frac{1}{2N}\left[\vartheta(x,\gamma) + \vartheta(x,\pi-\gamma) + \vartheta(x,2\gamma)\right]$$
$$= \rho(x) + \int_{-B}^{B} \vartheta(x-y,2\gamma)\rho_+(y)\,\mathrm{d}y, \tag{15}$$

where

$$2\pi\mathrm{i}\,\vartheta(x,\gamma) := \frac{2\mathrm{i}\sin\gamma}{\cosh 2x - \cos\gamma} = \frac{\mathrm{d}}{\mathrm{d}x}\ln\frac{\sinh(x+\mathrm{i}\gamma/2)}{\sinh(x-\mathrm{i}\gamma/2)}. \tag{16}$$

Equation (15) is a linear integral equation with two unknowns, B and ρ. In a first step, (15) is solved for $B=\infty$; in a second step, $\rho_+(x)$ is obtained depending on the parameter B and the dependence of B on the magnetic field h is calculated. We will see that $B=\infty$ corresponds to $h=0$, and a finite magnetic field $h>0$ induces a finite $B<\infty$. Finally, the susceptibility $\chi(h)$ is deduced. This procedure was first used by Takahashi for PBC and is reviewed in [18].

Note that in deriving (15) the range of definition of the involved functions has been enlarged. All functions in (15) are defined on $[-\infty,\infty]$; to calculate physical quantities (like the ground-state energy), however, we only need to know ρ_+, defined on $[-B,B]$. Actually, it will be shown later that instead of dealing with ρ_+, all quantities we are interested in can be expressed more conveniently by $g_+(x) := \theta(x)\rho(v+B)$. The calculation of these functions is done by Fourier transformation,

$$\rho(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\widetilde{\rho}(k)\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}k\;.$$

Let us first consider the case $B=\infty$, where $\rho\equiv\rho_+$. It is straightforward to solve (15) in Fourier space, where

$$\widetilde{\vartheta}(k,\gamma) = \frac{\sinh(\pi/2-\gamma/2)k}{\sinh\pi k/2}.$$

We denote the solution of (15) for $B=\infty$ by ρ_0 and find

$$\widetilde{\rho}_0(k) = \widetilde{s}(k) + \frac{1}{2N}\,\frac{\cosh\gamma k/4\,\cosh(\pi/4-\gamma/2)k}{\cosh\gamma k/2\,\cosh(\pi-\gamma)k/4}, \tag{17}$$

with

$$\widetilde{s}(k) := \frac{1}{2\cosh\gamma k/2},\;\; s(x) = \frac{1}{2\gamma\cosh\pi x/\gamma}.$$

Note that $\int_{-\infty}^{\infty}\rho(x)\mathrm{d}x = 1/2 + 1/(2N)$, in agreement with (14).

We now consider the case $B<\infty$, i.e., a finite magnetic field. Let us derive the equation that determines g_+. Using (17) we can rewrite (15) as

$$\rho(x) = \rho_0(x) + \int_{|y|>B}\kappa(x-y)\rho(y)\,\mathrm{d}y \tag{18}$$

$$\kappa(x) := \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\sinh(\pi/2-\gamma)k}{2\cosh\gamma k/2\,\sinh(\pi-\gamma)k/2}\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}k. \tag{19}$$

We now introduce the functions

$$\begin{aligned}&\rho(x+B) =: g(x) \equiv g_+(x) + g_-(x)\\&g_+(x) = \theta(x)g(x)\,, \qquad g_-(x) = \theta(-x)g(x)\,.\end{aligned} \tag{20}$$

Then $g(x)$ satisfies the equation

$$g(x) = \rho_0(x+B) + \int_0^\infty \kappa(x-y)g(y)\,\mathrm{d}y + \int_0^\infty \kappa(x+y+2B)g(y)\,\mathrm{d}y. \tag{21}$$

We seek a solution in the limit $B \gg 0$, which corresponds to $|h| \ll \alpha$, where α is some finite scale which is calculated later. The driving term $\rho_0(x+B)$ can be expanded in powers of $\exp[B]$. Since (21) is linear in g and ρ_0, we make the ansatz $g = g^{(1)} + g^{(2)} + \ldots$, where superscripts denote increasing powers of $\exp[B]$. Then

$$\begin{aligned}&g^{(1)}(x) = [\rho_0(x+B)]^{(1)} + \int_0^\infty \kappa(x-y)g^{(1)}(y)\,\mathrm{d}y\\&g^{(n)}(x) = [\rho_0(x+B)]^{(n)} + \int_0^\infty \kappa(x+y+2B)g^{(n-1)}(y)\,\mathrm{d}y + \int_0^\infty \kappa(x-y)g^{(n)}(y)\,\mathrm{d}y.\end{aligned}$$

Thus in each order, a linear integral equation of Wiener-Hopf-type has to be solved. This technique is explained for example in [19, 20]. It relies on the factorization of the kernel $\widetilde{\kappa}$,

$$1 - \tilde{\kappa} = 1/(G_+ G_-), \tag{22}$$

where G_+ (G_-) is analytical in the upper (lower) half plane and has asymptotics $\lim_{|k|\to\infty} G_\pm(k) = 1$. The functions $G_\pm$ are calculated in Appendix A. From (20), note that $\widetilde{g}_+$ ($\widetilde{g}_-$) is analytical in the upper (lower) half of the complex plane. Then

$$\widetilde{g}_+^{(1)}(k) = G_+(k)\left[\widetilde{\rho}_0(k)G_-(k)\mathrm{e}^{-\mathrm{i}kB}\right]_+^{(1)} \tag{23}$$

$$\begin{aligned}\widetilde{g}_+^{(2)}(k) = G_+(k)\Big\{&\left[\widetilde{\rho}_0(k)\,G_-(k)\,\mathrm{e}^{-\mathrm{i}kB}\right]_+^{(2)}\\&+\left[\widetilde{\kappa}(k)\,\widetilde{g}^{(1)}(-k)\,G_-(k)\,\mathrm{e}^{-2\mathrm{i}kB}\,G_-(k)\right]_+^{(2)}\Big\}\,,\end{aligned} \tag{24}$$

where

$$f_\pm(k) := \pm\frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty}\frac{f(q)}{k-q\pm\mathrm{i}\epsilon}\,\mathrm{d}q \tag{25}$$

is analytical in the upper (subscript $+$) or lower (subscript $-$) half of the complex plane such that $f = f_+ + f_-$. We will see later that it is sufficient to know $\widetilde{g}_+$. In this section we restrict ourselves to the calculation of $\widetilde{g}_+^{(1)}$. The calculation of $\widetilde{g}_+^{(2)}$ is sketched in Appendix B.

The bracket $[\ldots]_+^{(1)}$ in (23) is evaluated using (25), where only the pole nearest to the real axis is taken into account. Then we find

$$\widetilde{g}_+^{(1)}(k) = \left\{\begin{array}{l} G_+(k)\left\{\dfrac{a_0}{k+\mathrm{i}\pi/\gamma}\mathrm{e}^{-\pi/\gamma B}\right.\\[2ex] \left.+\dfrac{1}{2N}\left[\dfrac{a_1}{k+\mathrm{i}\pi/\gamma}\mathrm{e}^{-\pi B/\gamma} + \dfrac{b_1}{k+\mathrm{i}2\pi/(\pi-\gamma)}\mathrm{e}^{-2\pi B/(\pi-\gamma)}\right]\right\}\end{array}\right. \tag{26a}$$

for $\gamma \neq \pi/3$ and

$$\widetilde{g}_+^{(1)}(k) = G_+(k)\left[\frac{a_0}{k+\mathrm{i}3\pi}\mathrm{e}^{-3B} + \frac{1}{2N}\frac{c_1}{k+3\mathrm{i}}B\mathrm{e}^{-3B}\right] \tag{26b}$$

for $\gamma = \pi/3$ where the constants are given by

$$a_0 = \frac{\mathrm{i}}{\gamma} G_-(-\mathrm{i}\pi/\gamma) \tag{27a}$$

$$a_1 = \frac{\sqrt{2}\mathrm{i}}{\gamma} G_-(-\mathrm{i}\pi/\gamma) \frac{\sin \pi^2/(4\gamma)}{\cos(\pi^2/(4\gamma) - \pi/4)} \tag{27b}$$

$$b_1 = \frac{2\mathrm{i}}{\pi - \gamma} \tan \pi\gamma/(\pi - \gamma)\, G_-(-\mathrm{i}2\pi/(\pi - \gamma)) \tag{27c}$$

$$c_1 = \mathrm{i}\frac{18}{\pi^2} G_-(-3\mathrm{i}). \tag{27d}$$

For $\gamma = \pi/3$, terms $\mathrm{O}(B \exp[-B])$ occur in the boundary contribution which are absent for $\gamma = \pi/3$. These terms are leading compared to those $\mathrm{O}(\exp[-B])$ so that these latter have been neglected for the boundary contribution in (26*b*).

We are now ready to compute $s^z := S^z/N$ and $e := E/N$ from (9),(10):

$$s^z = 1/2 - \int_{-B}^{B} \rho_+(x)\mathrm{d}x + 1/(2N) \tag{28}$$

$$e = -hs^z - \frac{J \sin \gamma}{2} \int_{-B}^{B} \vartheta(x, \gamma)\rho_+(x)\mathrm{d}x + \frac{J}{4}\left(\cos \gamma + \frac{2 - \cos \gamma}{N}\right). \tag{29}$$

We insert (18) into (28) to obtain

$$s^z = \frac{\pi}{\pi - \gamma}\, \widetilde{g}_+(0), \tag{30}$$

which is an exact statement, including all orders $\widetilde{g}^{(n)}$. It is convenient to calculate $e - e_0$, where $e_0 := e(h = 0)$. We use again (18) which yields

$$\begin{aligned} e - e_0 &= -hs^z + \frac{4J\pi \sin \gamma}{\gamma} \int_0^\infty \frac{g_+(x)}{\cosh(x + B)\pi/\gamma}\, \mathrm{d}x \\ &= -\frac{h\pi}{\pi - \gamma}\left(\widetilde{g}_+^{(1)}(0) + \widetilde{g}_+^{(2)}(0)\right) + \frac{8\pi J \sin \gamma}{\gamma}\left[\left(\widetilde{g}_+^{(1)}(\mathrm{i}\pi/\gamma) + \widetilde{g}^{(2)}(\mathrm{i}\pi/\gamma)\right) \mathrm{e}^{-\pi B/\gamma} \right. \\ &\qquad \left. - \widetilde{g}_+^{(1)}(3\mathrm{i}\pi/\gamma)\mathrm{e}^{-3\pi B/\gamma} + \mathrm{O}\left(\mathrm{e}^{-3\pi B/\gamma}\widetilde{g}^{(2)}\right)\right], \end{aligned} \tag{31}$$

where in the last equation we restrict ourselves to the given orders. Now B is treated as a variational parameter and is determined in such a way that

$$\frac{\partial}{\partial B}(e - e_0) = 0. \tag{32}$$

In this section we consider only the leading order in (31). Inserting (26*a*), (30), (31) in (32), B is obtained as a function of h,

$$B = -\frac{\gamma}{\pi} \ln \frac{h}{\alpha} \tag{33}$$

$$\alpha := \frac{2\pi J \sin \gamma}{\gamma}(\pi - \gamma)\frac{G_+(\mathrm{i}\pi/\gamma)}{G_+(0)}\ . \tag{34}$$

Thus α sets the scale for h. The restriction to the leading orders in $\exp[-B]$ is equivalent to the leading orders in h in the limit $|h| \ll \alpha$.

One now makes use of (34) to determine $s^z(h)$ from (30), and therefrom $\chi(h) = \partial s^z/\partial h$. Inserting the explicit expressions for $G_\pm$ from Appendix A we find

$$\chi_{\mathrm{bulk}} = \frac{\gamma}{(\pi - \gamma)\pi J \sin \gamma}\ . \tag{35a}$$

The boundary contribution is given by

$$\chi_B(h) = \begin{cases} \dfrac{\gamma}{J(\pi-\gamma)\pi\sqrt{2}\,\sin\gamma}\,\dfrac{\sin\pi^2/(4\gamma)}{\cos(\pi^2/(4\gamma)-\pi/4)} \\ +\dfrac{2\gamma\sqrt{\pi}}{(\pi-\gamma)^2}\tan\dfrac{\pi\gamma}{\pi-\gamma}\dfrac{1}{\alpha}\,\dfrac{\Gamma\left(\pi/(\pi-\gamma)\right)}{\Gamma\left(1/2+\gamma/(\pi-\gamma)\right)}\,(h/\alpha)^{-(\pi-3\gamma)/(\pi-\gamma)} \end{cases} \tag{35b}$$

for $\gamma \neq \pi/3$ with

$$\alpha = 2J(\pi-\gamma)\sqrt{\pi}\,\frac{\sin\gamma}{\gamma}\,\frac{\Gamma(1+\pi/(2\gamma))}{\Gamma(1/2+\pi/(2\gamma))} \tag{35c}$$

and by

$$\chi_B(h) = -\frac{1}{\sqrt{3}\pi^2}\left(\ln\frac{4\,h}{27\pi}+1\right) \tag{35d}$$

for $\gamma = \pi/3$. Note that the first term in (35b), which is independent of magnetic field h, is the leading contribution for $\gamma > \pi/3$ (pole closest to the real axis in (23)). For $\gamma < \pi/3$ the second term dominates and, in addition, this term is the next-leading contribution for $\gamma > \pi/3$ (second pole in (23)). For $\pi/7 < \gamma < \pi/3$ the constant term represents the next-leading contribution, however, for $\gamma < \pi/7$ a pole at $6\pi\mathrm{i}/(\pi-\gamma)$ in (23) becomes second nearest to the real axis and gives the next-leading contribution (see Appendix B).

The second term in (35b) is in perfect agreement with the result obtained by conformal field theory and bosonization in [11, 12]. However, the first, field independent term has not been obtained before. Also the result (35d) for the special case $\gamma = \pi/3$ is new. Our results are in qualitative agreement with the TBA-work [7] at $T = 0$, where also a finite value of $\chi_B(T = 0, h = 0)$ for $\gamma > \pi/3$ (i.e. $\Delta < 1/2$) and a divergent contribution with the same exponent as in (35b) for $\gamma < \pi/3$ ($\Delta > 1/2$) have been found. However, the coefficients in (35b) differ from those in [7], due to an incorrect treatment of the Bethe root at spectral parameter $x = 0$ in [7] (c.f. the discussion in section 1).

3.2. Isotropic case

The isotropic case $\gamma = 0$ (i.e. $\Delta = 1$) is treated in the same manner as the anisotropic case $\gamma \neq 0$. For the bulk susceptibility, (35a), the limit $\gamma \to 0$ can be performed directly, yielding $\chi_{\text{bulk}} = 1/J\pi^2$. For the boundary contribution this limit is more complicated and we describe the procedure in the following.

First, we rescale (9) by $\lambda_j \to \gamma\lambda_j$. This is equivalent to substituting $k \to k/\gamma$ in Fourier space. Then

$$\begin{aligned} \widetilde{s}(k) &= \frac{1}{2\cosh k/2} \\ \widetilde{\rho}_0(k) &= \widetilde{s}(k) + \frac{1}{2N}\,\frac{1}{2\cosh k/2}\left(1+\mathrm{e}^{-|k|/2}\right)\,. \end{aligned} \tag{36}$$

Whereas the analyticity properties of the bulk contribution to (36) are qualitatively the same as in (17), the boundary contribution shows, besides poles, a cut along the imaginary axis. In (23), the $[\ldots]_+$-bracket thus yields contributions $\mathrm{O}(\exp[-const.\,B])$ from the poles, and algebraic contributions due to the cut. The exponential contributions are clearly sub-leading in comparison to the algebraic ones, so only the

latter are calculated in the following. Using eq. (A.2) from Appendix A and explicit expressions for $G_\pm(k)$, we find (omitting the bulk contribution)

$$\widetilde{g}_+^{(1)}(k) = \begin{cases} G_+(0)(\alpha_1/B + \alpha_2(\ln B)/B^2 + \alpha_3/B^2) & \\ +\mathrm{O}((\ln B)/B^3, 1/B^3), & k=0 \\ \mathrm{i}\alpha_1 G_+(k)/(kB^2), & k \neq 0 \end{cases}$$

$$\alpha_1 = \frac{1}{\sqrt{2}\pi}\,,\ \alpha_2 = -\frac{\sqrt{2}}{4\pi^2}\,,\ \alpha_3 = \frac{1}{\sqrt{2}\pi^2}\left(\ln 2 - \frac{1}{2}\ln(2\pi)\right)\,.$$

From (30), (31), (32) we obtain

$$B = -\frac{1}{\pi}\ln\frac{h}{\alpha} \tag{37}$$

$$\alpha^{-1} = \frac{G_+(0)}{2\pi J G_+(\mathrm{i}\pi)}\,. \tag{38}$$

These equations are obtained by those from the anisotropic case, (33), (34), by scaling $B \to \gamma B$ and sending $\gamma \to 0$ afterwards. Carrying out the same steps which lead to (35*b*), one finds the boundary contribution

$$s_B^z(h) = -\frac{1}{4}\left(\frac{1}{\ln h/h_0} + \frac{\ln|\ln h/h_0|}{2\ln^2 h/h_0}\right) + \mathrm{o}(\ln^{-2} h) \tag{39}$$

$$\chi_B(h) = \frac{1}{4}\left(\frac{1}{h\ln^2 h/h_0} + \frac{\ln|\ln h/h_0|}{h\ln^3 h/h_0} - \frac{1}{2h\ln^3 h/h_0}\right) + \mathrm{o}\left(\frac{1}{h\ln^3 h}\right) \tag{40}$$

$$h_0 = \alpha/\sqrt{2} = J\pi\sqrt{\pi/\mathrm{e}}\,. \tag{41}$$

The scale h_0 has been chosen such that in (39), no terms $\mathrm{O}(\ln^{-2} h)$ occur. The results (40), (41) agree with the TBA-work by Frahm et al. [15] for $T = 0$. Furthermore, agreement is found with [11, 12, 9], where scales which differ from ours (41) by a constant factor were used.

3.3. Numerical evaluation

To obtain results for the case when $|h| \not\ll \alpha$, (15) has to be solved numerically. For this purpose the bulk and boundary contributions to $\rho(x)$ in equation (15) are treated separately. Both can be evaluated numerically for arbitrary values of B. The corresponding value for h is then derived from the minimum condition (32). This finally yields $s^z(h)$ and therefrom $\chi(h)$, c.f. eq. (28). The result for the bulk susceptibility is shown in fig. 2, together with the $h = 0$ values (35*a*). The boundary susceptibility is shown in fig. 3 (4) for $\Delta < 1/2$ ($\Delta > 1/2$). In both cases, the numerical solution confirms the analytical findings in the limit $|h| \ll \alpha$.

4. Finite temperatures

In the preceding section we calculated ground-state properties by making use of the integrability of the Hamiltonian (1) with $J_1' = J_2' = 0$. The next step would be to exploit integrability in order to calculate finite-temperature properties. However, the TBA seems to be problematic for systems with OBC as discussed in the introduction. The other available technique, namely the quantum-transfer-matrix-approach (QTM) [21], has not been applied to open systems so far. The problem to modify the TBA

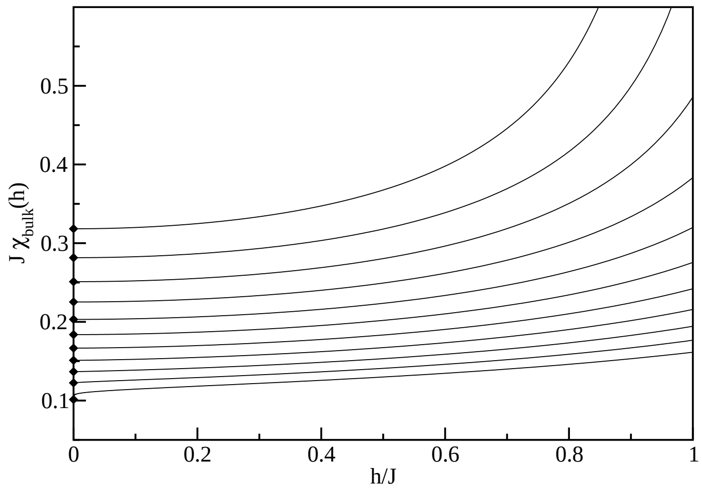

Figure 2. Bulk susceptibility from a numerical solution of eq. (15). The diamonds denote the $h = 0$ values according to ($35a$). Note that the $h = 0$ value is approached with infinite slope in the isotropic case due to logarithmic terms, cf. eq. (B.17).

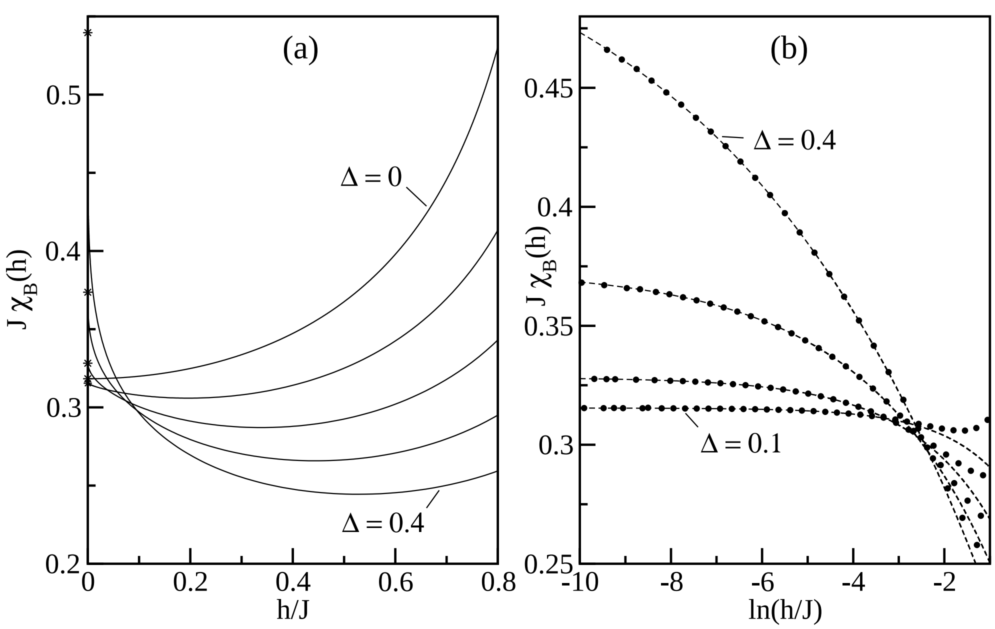

Figure 3. (a) $\chi_B(h)$ for $\Delta = 0.0, \cdots, 0.4$. The stars denote the $h = 0$ values according to eq. ($35b$). (b) Comparison between the numerical solution (dots) of eq. (15) and the asymptotics (dashed lines) for $|h| \ll \alpha$ (eq. ($35b$)).

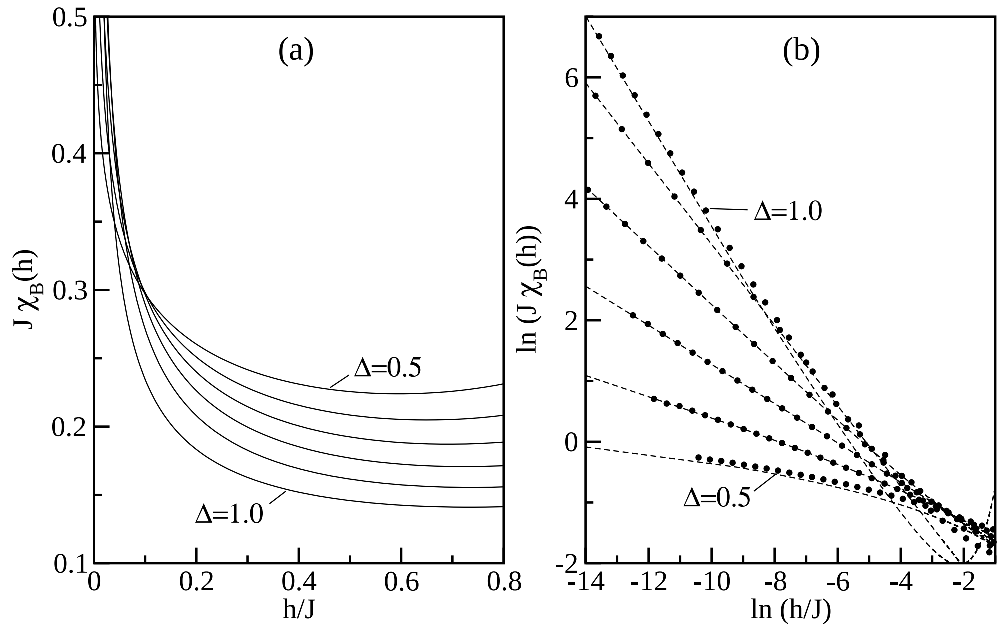

Figure 4. (a) $\chi_B(h)$ for $\Delta = 0.5, \cdots, 1.0$. (b) Comparison between the numerical solution (dots) of eq. (15) and the asymptotics (dashed lines) for $|h| \ll \alpha$ (eq. (35*b*)).

appropriately for OBC (if it is applicable at all) and the challenge to apply the QTM-method for OBC remain open issues for future research. Here, we use field theoretical arguments combined with a numerical study to discuss finite temperatures.

First, we want to present a way different from section 3 to calculate the boundary susceptibility. Because translational invariance is broken in a system with OBC the one-point correlation function $\langle S^z(r)\rangle$ is no longer a constant. The *excess magnetization* caused by the boundary can be defined as

$$M_{\rm exc}(r) = \langle S^z(r)\rangle_{\rm OBC} - M_{\rm PBC} \tag{42}$$

where $M_{\rm PBC}$ is the magnetization per site in the system with PBC and r is the distance from the boundary. The local boundary susceptibility is then given by $\chi_B(r) = \partial M_{\rm exc}(r)/\partial h$ and the total boundary susceptibility χ_B can be obtained by

$$\chi_B = \sum_{r=1}^{\infty} \chi_B(r) = \chi_{\rm OBC} - \chi_{\rm PBC}\,. \tag{43}$$

This means that we can calculate χ_B by considering only a local quantity which is particularly useful in numerical calculations where it is difficult to obtain the $1/N$ contribution directly. Particularly suited for this purpose is the density-matrix renormalization group applied to transfer matrices (TMRG) because the thermodynamic limit is performed exactly. The idea of the TMRG is to express the partition function Z of a one-dimensional quantum model by that of an equivalent two-dimensional classical model which can be derived by the Trotter-Suzuki formula [22, 23]. For the classical model a suitable transfer matrix T can be defined which

allows for the calculation of all thermodynamic quantities in the thermodynamic limit by considering solely the largest eigenvalue of this transfer matrix. Details of the algorithm can be found in Refs. [24, 25, 26, 27]. The method has been extended to impurity problems in [28]. In particular, the local magnetization at a distance r from the boundary of a system with N sites is given by

$$\langle S^z(r)\rangle = \frac{\sum_n \langle \Psi_L^n | T(S^z) T^{r-1} \widetilde{T} T^{N-r-1} | \Psi_R^n \rangle}{\sum_n \langle \Psi_L^n | T^{N-1} \widetilde{T} | \Psi_R^n \rangle} \tag{44}$$

where $|\Psi_R^n\rangle$ ($\langle \Psi_L^n|$) are the right (left) eigenstates of the transfer matrix T, $\widetilde{T}$ is a modified transfer matrix containing the broken bond and $T(S^z)$ is the transfer matrix with the operator S^z included. Because the spectrum of T has a gap between the leading eigenvalue Λ_0 and the next-leading eigenvalues, eq. (44) reduces in the thermodynamic limit to

$$\lim_{N\to\infty} \langle S^z(r)\rangle = \frac{\langle \Psi_L^0 | T(S^z) T^{r-1} \widetilde{T} | \Psi_R^0 \rangle}{\Lambda_0^r \langle \Psi_L^0 | \widetilde{T} | \Psi_R^0 \rangle} \ . \tag{45}$$

Therefore only the leading eigenvalue and the corresponding eigenvectors have to be known to calculate the local magnetization in the thermodynamic limit. Far away from the boundary $\langle S^z(r)\rangle$ becomes a constant, the bulk magnetization

$$\begin{aligned} m = \lim_{r\to\infty} \lim_{N\to\infty} \langle S^z(r)\rangle &= \lim_{r\to\infty} \frac{\sum_n \langle \Psi_L^0 | T(S^z) T^{r-1} | \Psi_R^n \rangle \langle \Psi_L^n | \widetilde{T} | \Psi_R^0 \rangle}{\Lambda_0^r \langle \Psi_L^0 | \widetilde{T} | \Psi_R^0 \rangle} \\ &= \frac{\langle \Psi_L^0 | T(S^z) | \Psi_R^0 \rangle}{\Lambda_0} \ . \end{aligned} \tag{46}$$

To obtain numerically the susceptibility profile $\chi_B(r)$ at $h = 0$ we calculate $M_{\mathrm{exc}}(r)$ for small fields $h/J \sim 10^{-2}$ to 10^{-3} by using eqs. (45,46) and taking the numerical derivative. As an example we show in fig. 5 the susceptibility profile for $\Delta = 0.6$ at various temperatures.

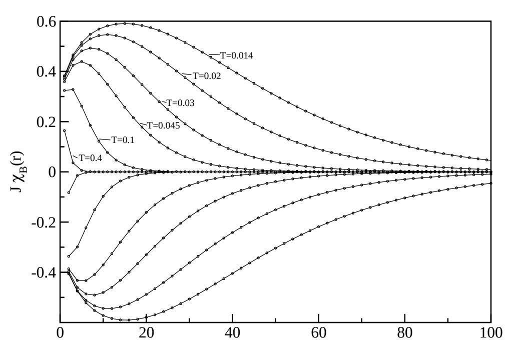

Figure 5. Susceptibility profile for $\Delta = 0.6$. The lines are a guide to the eye.

At sufficiently low temperatures the susceptibility profile exhibits a maximum. This maximum gets shifted further away from the boundary as the temperature is lowered. The dependence of $\chi_B(r)$ on Δ at fixed temperature is shown in Fig. 6. Here the maximum becomes more pronounced with increasing Δ and is at the same time shifted further into the chain.

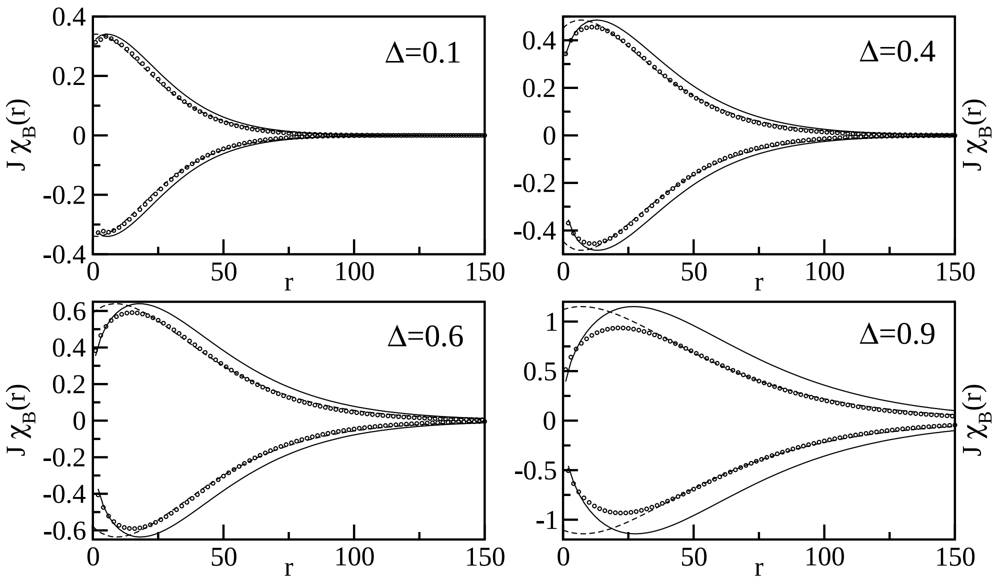

Figure 6. Susceptibility profiles for different Δ at $T/J = 0.01387$. The TMRG data are denoted by circles, the lines are the field theory results according to Eq. (51) and the dashed lines the field theory results shifted by some lattice spacings (see text below).

Next we want to compare the numerics with field theory predictions. We start with the bulk two-point correlation function $\langle S^z(r)S^z(0)\rangle$. The leading term in the long distance asymptotics of this function at zero temperature is known to be given by [29, 30, 31, 32, 33]

$$\langle S^z(r)S^z(0)\rangle \sim A\frac{\cos(2k_F r+\phi)}{r^{2x}} \tag{47}$$

with an amplitude A and phase ϕ. The Fermi momentum is given by $k_F = \pi(1\pm 2m)/2$ and the scaling dimension by $x = K/2$. The usual mapping of the complex plane onto a semi-infinite cylinder then implies for small temperatures

$$\langle S^z(r)S^z(0)\rangle \sim A\frac{\cos(2k_F r+\phi)}{\left(\frac{v_s}{\pi T}\sinh\frac{\pi T r}{v_s}\right)^K} \;. \tag{48}$$

Using Cardy's relation between $2n$-point functions in the bulk and n-point functions near a surface [2] one can now directly obtain the magnetization near the boundary

$$\langle S^z(r)\rangle \sim \widetilde{A}\frac{\cos(2k_F r+\widetilde{\phi})}{\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T r}{v_s}\right)^{K/2}} \;. \tag{49}$$

Note that although the critical exponent is only half the exponent appearing in the two-point bulk correlation function both decay exponentially with exactly the same correlation length $\xi = v_s/(2\pi x T)$. With the known result for the bulk susceptibility $\chi_{\text{bulk}}(h=0) = K/2\pi v_s$ we obtain

$$\langle S^z(r)\rangle \quad \sim \widetilde{A}\frac{(-1)^r\sin(Khr/v_s)}{\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T r}{v_s}\right)^{K/2}} \quad \text{for } h\ll 1 \text{ and}$$

$$\chi_B(r)|_{h=0} \sim \frac{\widetilde{A}K}{v_s} \frac{(-1)^r\, r}{\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T r}{v_s}\right)^{K/2}} \,. \tag{50}$$

This is the leading contribution to the boundary susceptibility. Note that eq. (50) agrees for the special case $\Delta = 1$ with the result given in [1]. The amplitude depends only on the operator product expansion of S^z and is given by $\widetilde{A} = \sqrt{A_z/2}$ where A_z has been derived by Lukyanov and Terras [33] (see eq. (4.3)). However, this alternating term does not contribute when calculating χ_B by integrating over all lattice sites. The leading non-oscillating contribution has already been obtained by Fujimoto and Eggert [11] and Furusaki and Hikihara [12]. Including this term we find for the susceptibility profile

$$\begin{aligned}\chi_B(r)|_{h=0} \sim \sqrt{\frac{A_z}{2}}\frac{K}{v_s} \frac{(-1)^r\, r}{\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T r}{v_s}\right)^{K/2}} \\ + \frac{4K^2\lambda}{v_s^2}\frac{r^2}{\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T r}{v_s}\right)^{2K}}\end{aligned} \tag{51}$$

where the amplitude λ is given in [33, 12]. This field theory result is shown as straight lines in Fig. 6 in comparison to the numerics. For all Δ the shape of the curves agrees well with the numerical results. However, especially at larger Δ the height of the maximum is overestimated and there is also a shift by a few lattice sites. When we shift the theoretical curves by an appropriate amount of lattice spacings (dashed lines in Fig. 6) we see that the predicted exponential decay for larger distances agrees perfectly with the numerical data.

First, we should note that we cannot expect that the field theoretical treatment yields reliable results for short distances. In addition, the next-leading alternating terms in the asymptotic expansion of the bulk two-point correlation function will become more and more important as $\Delta \to 1$ [33]. This makes our approximation to take only the leading term (47) into account apparently worse for larger Δ. In fact shifting the field theoretical result is equivalent to taking contributions with larger scaling dimensions into account. Our observation that the shift increases with increasing Δ is therefore consistent with the increasing importance of next-leading terms. We also want to mention that a similar shift has been observed before for the isotropic case [1].

Finally we want to discuss the total boundary susceptibility χ_B at finite temperature. To calculate it numerically we have in principle to sum $\chi_B(r)$ over all lattice sites. However, at the lowest considered temperature the correlation length $\xi < 50$ and it is sufficient to take the sum over the first 200 sites around the boundary. The results for $\Delta = 0.1 - 0.4$ are shown in Fig. 7 and for $\Delta = 0.6 - 0.9$ in Fig. 8. For the low-temperature asymptotics we already know from our Bethe ansatz calculations that there is a temperature and magnetic field independent term which dominates for $\Delta < 0.5$. In addition there is a temperature dependent contribution which stems from the integral over all lattice sites of the non-oscillating term in eq. (51) and dominates for $\Delta > 0.5$. This integral has already been calculated in [11, 12], yielding the leading temperature-dependent contribution to $\chi_B(T)$. However, the constant term cannot be calculated within the field-theoretical framework. Our knowledge of this term from the BA calculations in the previous section allows us to obtain a low-temperature

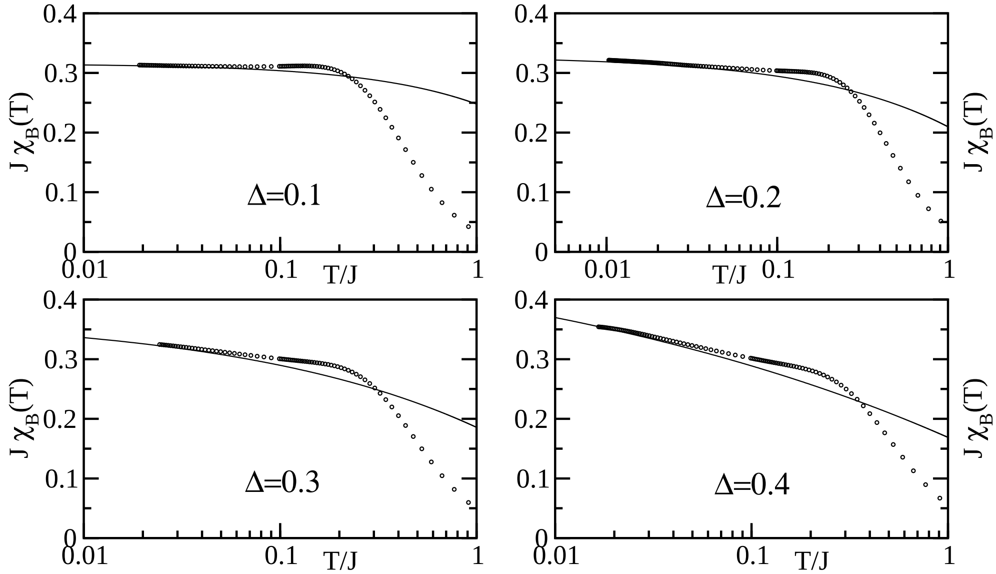

Figure 7. Comparison between TMRG (circles) and the low-temperature asymptotics (lines) according to (52) for $\Delta = 0.1, \cdots, 0.4$.

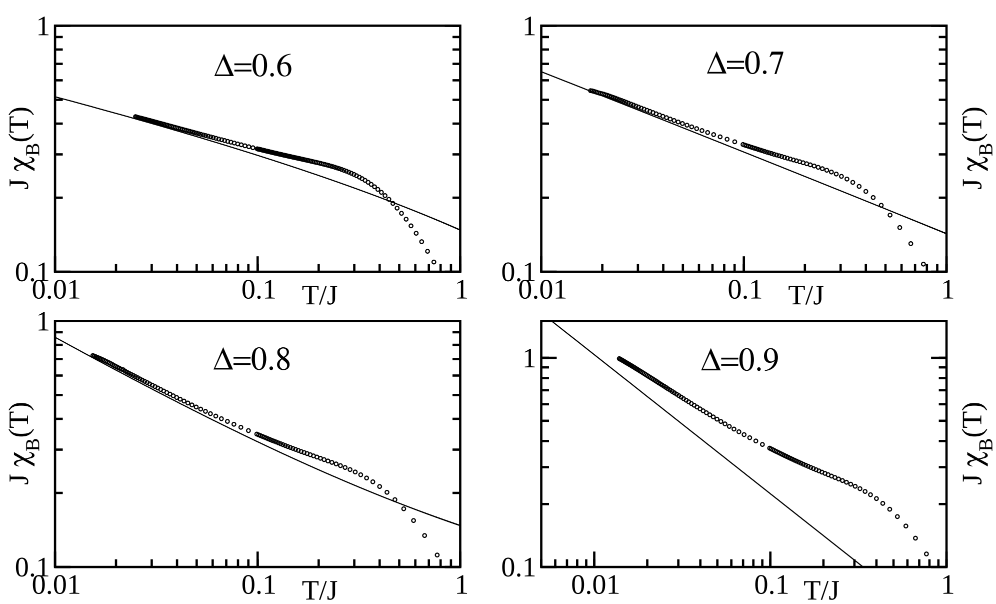

Figure 8. Same as fig. 7 with $\Delta = 0.6, \cdots, 0.9$.

asymptotics which is valid for all $0 \leq \Delta < 1$. This asymptotics is given by

$$\chi_B(T, h=0) = \frac{K-1}{J\sqrt{2}\pi \sin(K-1)} \frac{\sin\frac{\pi}{4}\frac{K}{K-1}}{\cos\frac{\pi}{4}\frac{1}{K-1}} + \lambda \frac{K\Gamma(K)\Gamma(3-2K)(\pi^2 - 2\Psi'(K))}{4v^2(2-1/K)\Gamma(2-K)} \left(\frac{2\pi T}{v}\right)^{2K-3} \tag{52}$$

where $\Psi'(x) = \mathrm{d}^2 \ln\Gamma(x)/\mathrm{d}x^2$. The first term is our BA result, eq. (35b), where we have substituted $\gamma = \pi(K-1)/K$. The second term is the leading temperature dependent contribution taken from [11, 12]. As in the case $h \neq 0$, $T = 0$, we expect that these are the leading and the sub-leading contributions for $\Delta \lesssim 0.9$. For larger Δ we expect that other temperature dependent terms will become more important than the constant term and we have to omit it in this case to stay consistent. Note that the leading temperature dependent term has the same exponent $2K-3$ as the leading magnetic field dependent term in eq. (35b). This is consistent with scaling arguments. The lines in figs. 7,8 denote the low-T asymptotics according to this formula and are in excellent agreement with the numerics except for $\Delta = 0.9$ where the asymptotic limit at the lowest considered T is not yet reached. However, this is expected due to the afore mentioned other temperature dependent terms which will become sub-leading for $\Delta \gtrsim 0.9$ and even equally important as the term with exponent $2K-3$ for $\Delta \to 1$, yielding finally a logarithmic dependence on temperature [11, 12].

5. Conclusions

In the first part we have calculated the boundary contribution to the magnetic susceptibility of the XXZ-chain with OBC at zero temperature and finite magnetic field by BA. For small magnetic fields and $\gamma < \pi/3$ ($\Delta > 1/2$) the BA result for the leading divergent term agrees with the field theoretical analysis [11, 12]. For $\gamma > \pi/3$ ($\Delta < 1/2$) a field independent term is dominating. This term has not been obtained before. We also derived for the first time the leading term for the special case $\gamma = \pi/3$ ($\Delta = 1/2$). In addition we have presented a numerical solution of the BA equations for arbitrary field h. We used the numerics for a verification of our analytical results for $|h| \ll \alpha$.

In the second part we have calculated numerically susceptibility profiles near the boundary by the TMRG method and compared these results with a low-temperature asymptotics which we obtained by field theoretical methods. Apart from a shift by a few lattice sites we have found good agreement. By combining a temperature and magnetic field independent term, which we obtained by BA and which is dominating for $\Delta < 1/2$, with the leading temperature dependent term, which has been calculated in [11, 12] and dominates for $\Delta > 1/2$, we have obtained a low-temperature asymptotics for $\chi_B(T)$ which is valid for all $0 \leq \Delta < 1$. Numerically, $\chi_B(T)$ has been obtained by a summation of $\chi_B(r, T)$ over a sufficient number of sites around the boundary. At low-temperatures excellent agreement with the analytical formula was found. The remaining challenge is to calculate the finite-temperature properties analytically by using the integrability of the model, either by TBA or by the QTM-method.

We acknowledge very helpful discussions with Andreas Klümper, Ian Affleck and Frank Göhmann.

Appendix A. Factorization of the kernel

Let us first carry out the factorization (22) for the anisotropic case

$$\begin{aligned}\frac{1}{G_+(k)\,G_-(k)} &= \frac{\sinh \pi k/2}{2\cosh\gamma k/2\,\sinh(\pi-\gamma)k/2}\\ G_-(k) &= G_+(-k).\end{aligned}$$

Using properties of the Γ function, we find

$$\begin{aligned}G_+(k) &= \sqrt{2(\pi-\gamma)}\frac{\Gamma(1-\mathrm{i}k/2)}{\Gamma(1/2-\mathrm{i}\gamma k/(2\pi))\,\Gamma(1-\mathrm{i}k(\pi-\gamma)/(2\pi))}\,\mathrm{e}^{-\mathrm{i}ak}\\ a &= \frac{1}{2}\left[\frac{\gamma}{\pi}\ln(\pi/\gamma-1)-\ln(1-\gamma/\pi)\right],\end{aligned}$$

where a is determined such that $\lim_{|k|\to\infty} G_\pm(k)=1$.

As already mentioned in section 3.2, the isotropic limit is realized by scaling $k\to k/\gamma$, thus for $\gamma=0$,

$$\frac{1}{G_+(k)\,G_-(k)} = \frac{\mathrm{e}^{|k|/2}}{2\cosh k/2}. \tag{A.1}$$

By making use of

$$-\frac{|k|}{2} = \frac{\mathrm{i}k}{2\pi}\ln\mathrm{i}k - \frac{\mathrm{i}k}{2\pi}\ln(-\mathrm{i}k), \tag{A.2}$$

the exponential in (A.1) is factorized in functions analytical in the upper and lower half planes with

$$\begin{aligned}G_+(k) &= \sqrt{2\pi}\frac{(-\mathrm{i}k)^{-\mathrm{i}k/(2\pi)}}{\Gamma(1/2+\mathrm{i}k/(2\pi))}\,\mathrm{e}^{-\mathrm{i}ak}\\ a &= -\frac{1}{2\pi}-\frac{\ln(2\pi)}{2\pi}.\end{aligned}$$

Appendix B. Next-leading orders

Our focus here is on the anisotropic case; we comment on the isotropic case at the end of this appendix.

The calculation of the next-leading order, i.e. of $\tilde{g}^{(2)}$ in (24), is technically more involved than the leading order $\tilde{g}^{(1)}$, because there are *two* contributions in (24). The calculation is done following the same steps as in section 3, so that we merely give the results here.

The $[\cdots]_+$-brackets in (24) are evaluated using the integral representation (25). Now, the pole next-nearest to the real axis is taken into account in the first summand in (24). The second term already contains a factor $\exp[-2\mathrm{i}kB]$, so that the pole next to the real axis yields the leading contribution. Thus we find for $\gamma\neq\pi/3$

$$\begin{aligned}\tilde{g}_+^{(2)}(k) &= G_+(k)\\ &\times\left\{\left(\frac{a_{0,1}}{k+\mathrm{i}3\pi/\gamma}+\frac{a_{0,2}}{k+\mathrm{i}\pi/\gamma}\right)\mathrm{e}^{-3\pi B/\gamma}+\frac{a_{0,3}}{k+\mathrm{i}2\pi/(\pi-\gamma)}\,\mathrm{e}^{-(\pi/\gamma+4\pi/(\pi-\gamma))B}\right.\\ &+\frac{1}{2N}\left[\left(\frac{a_{1,1}}{k+\mathrm{i}3\pi/\gamma}+\frac{a_{1,2}}{k+\mathrm{i}\pi/\gamma}\right)\mathrm{e}^{-3\pi B/\gamma}+\frac{a_{1,3}}{k+\mathrm{i}2\pi/(\pi-\gamma)}\,\mathrm{e}^{-(\pi/\gamma+4\pi/(\pi-\gamma))B}\right.\\ &+\left(\frac{b_{1,1}}{k+\mathrm{i}6\pi/(\pi-\gamma)}\right.\end{aligned}$$

$$+\frac{b_{1,3}}{k+\mathrm{i}2\pi/(\pi-\gamma)}\Bigg)\,\mathrm{e}^{-6\pi/(\pi-\gamma)B}+\frac{b_{1,2}}{k+\mathrm{i}\pi/\gamma}\mathrm{e}^{-2(\pi/\gamma+\pi/(\pi-\gamma))B}\Bigg]\Bigg\} \tag{B.1}$$

$$a_{0,1}=-\frac{\mathrm{i}}{\gamma}\,G_-\left(-\mathrm{i}\frac{3\pi}{\gamma}\right) \tag{B.2}$$

$$a_{0,2}=\frac{\mathrm{i}}{2\gamma\pi}\,\tan\frac{\pi^2}{2\gamma}\,G_-^3\left(-\mathrm{i}\frac{\pi}{\gamma}\right) \tag{B.3}$$

$$a_{0,3}=\frac{\mathrm{i}}{\pi(\pi+\gamma)}\,\tan\frac{\pi\gamma}{\pi-\gamma}\,G_-\left(-\mathrm{i}\frac{\pi}{\gamma}\right)\,G_-^2\left(-\mathrm{i}\frac{2\pi}{\pi-\gamma}\right) \tag{B.4}$$

$$a_{1,1}=\mathrm{i}\frac{2\,\sin\pi/4\,\sin3\pi^2/(4\gamma)}{\gamma\,\cos(3\pi^2/(4\gamma)+\pi/4)}\,G_-\left(-\mathrm{i}\frac{3\pi}{\gamma}\right) \tag{B.5}$$

$$a_{1,2}=\frac{a_1}{2\pi}\tan\frac{\pi^2}{2\gamma}G_-^2\left(-\mathrm{i}\frac{\pi}{\gamma}\right) \tag{B.6}$$

$$a_{1,3}=\frac{a_1\gamma}{\pi(\pi+\gamma)}\,\tan\frac{\pi\gamma}{\pi-\gamma}\,G_-^2\left(-\mathrm{i}\frac{2\pi}{\pi-\gamma}\right) \tag{B.7}$$

$$b_{1,1}=\mathrm{i}\frac{2}{\pi-\gamma}\,\tan\frac{3\gamma\pi}{\pi-\gamma}\,G_-\left(-\mathrm{i}\frac{6\pi}{\pi-\gamma}\right) \tag{B.8}$$

$$b_{1,2}=\frac{b_1(\pi-\gamma)}{\pi(\pi+\gamma)}\,\tan\frac{\pi^2}{2\gamma}\,G_-^2\left(-\mathrm{i}\frac{\pi}{\gamma}\right) \tag{B.9}$$

$$b_{1,3}=\frac{b_1}{4\pi}\,\tan\frac{\pi\gamma}{\pi-\gamma}\,G_-^2\left(-\mathrm{i}\frac{2\pi}{\pi-\gamma}\right), \tag{B.10}$$

and for $\gamma=\pi/3$

$$\widetilde{g}_+^{(2)}(k)=G_+(k)\left\{\frac{a_{0,4}}{k+3\mathrm{i}}\,B\,\mathrm{e}^{-9B}+\frac{1}{2N}\left[\frac{c_{1,1}}{k+9\mathrm{i}}B\mathrm{e}^{-9B}+\frac{c_{1,2}}{k+3\mathrm{i}}B^2\mathrm{e}^{-9B}\right]\right\} \tag{B.11}$$

$$a_{0,4}=\mathrm{i}\frac{9}{\pi^3}G_-^3(-3\mathrm{i})\,,\ c_{1,1}=\mathrm{i}\frac{18}{\pi^2}\,G_-(-9\mathrm{i})\,,\ c_{1,2}=\frac{3\,c_1}{\pi^2}\,G_-^2(-3\mathrm{i}).$$

This expression for $\widetilde{g}_2$ is inserted into (31), where we now have to keep all the indicated terms.‖ Then B as a function of h is derived. In section 3, we found that this relationship is the same both for the boundary and for the bulk in the leading order. This is no longer true when next-leading terms are considered. For the bulk we obtain

$$\alpha\mathrm{e}^{-\pi B/\gamma}=h\left(1+A_1\left(\frac{h}{\alpha}\right)^2+A_2\left(\frac{h}{\alpha}\right)^{4\gamma/(\pi-\gamma)}+\left[\frac{1}{3}\,\frac{a_{0,4}}{a_0}\left(\frac{h}{\alpha}\right)^2\ln\frac{h}{\alpha}\right]_{\gamma=\pi/3}\right) \tag{B.12}$$

$$A_1=\frac{a_{0,2}}{a_0}+\frac{G_-(-\mathrm{i}3\pi/\gamma)}{G_-(-\mathrm{i}\pi/\gamma)}\,,\ A_2=\frac{\pi-\gamma}{2\gamma}\,\frac{a_{0,3}}{a_0}$$

and for the boundary

$$\alpha\mathrm{e}^{-\pi B/\gamma}=h\left(1+A_1\left(\frac{h}{\alpha}\right)^2+A_2\left(\frac{h}{\alpha}\right)^{4\gamma/(\pi-\gamma)}+B_1\left(\frac{h}{\alpha}\right)^{-1+6\gamma/(\pi-\gamma)}\right.$$

$$\left.+B_2\left(\frac{h}{\alpha}\right)^{1+2\gamma/(\pi-\gamma)}+\left[\frac{c_{1,2}}{3a_1}\left(\frac{h}{\alpha}\right)^2\ln^2\frac{h}{\alpha}+\frac{c_1}{3}\,\frac{G_-(-9\mathrm{i})}{G_-(-3\mathrm{i})}\left(\frac{h}{\alpha}\right)^2\ln\frac{h}{\alpha}\right]_{\gamma=\pi/3}\right) \tag{B.13}$$

‖ It is indeed sufficient to restrict the expansion of the $1/\cosh(x+B)$-factor in (31) to the first two orders. The next term would involve the exponent $5\pi/\gamma$. Comparing with the largest exponent in (B.1), $5\pi/\gamma>\pi/\gamma+4\pi/(\pi-\gamma)$ for $\gamma<\pi/2$. However, $\gamma=\pi/2$ is allowed, since in this case, all coefficients except $a_{0,1}$, $a_{1,1}$ vanish.

$$A_1 = \frac{a_{1,2}}{a_1} + \frac{G_-(-\mathrm{i}3\pi/\gamma)}{G_-(-\mathrm{i}\pi/\gamma)}\,,\; A_2 = \frac{\pi-\gamma}{2\gamma}\,\frac{a_{1,3}}{a_1}$$

$$B_1 = \frac{2(\pi-\gamma)}{\pi+\gamma}\,\frac{b_{1,3}}{a_1}\,,\; B_2 = \frac{\pi+\gamma}{2(\pi-\gamma)}\,\frac{b_{1,2}}{a_1} + \frac{G_-(-\mathrm{i}3\pi/\gamma)}{G_-(-\mathrm{i}\pi/\gamma)}\,\frac{b_1}{a_1}.$$

In (B.12), (B.13) and in the following, for $\gamma = \pi/3$ the only nextleading terms are those labeled by $[\ldots]_{\gamma=\pi/3}$. Combining these equations with (30), one finds

$$\begin{aligned} s^z_{\mathrm{bulk}}(h) = \sqrt{\frac{2}{\pi(\pi-\gamma)}}\Bigg\{ & G_-(-\mathrm{i}\pi/\gamma)\frac{h}{\alpha} \\ & + \left(\frac{1}{\pi}\tan\frac{\pi^2}{2\gamma}\,G_-^3\left(-\mathrm{i}\frac{\pi}{\gamma}\right) - \frac{1}{3}G_-\left(-\mathrm{i}\frac{3\pi}{\gamma}\right) + \frac{G_+(\mathrm{i}3\pi/\gamma)G_+(\mathrm{i}\pi/\gamma)}{G_+(0)}\right)\left(\frac{h}{\alpha}\right)^3 \\ & + \frac{\pi-\gamma}{\pi(\pi+\gamma)}\,\tan\frac{\pi\gamma}{\pi-\gamma}\,G_-\left(-\mathrm{i}\frac{\pi}{\gamma}\right)\,G_-^2\left(-\mathrm{i}\frac{2\pi}{\pi-\gamma}\right)\left(\frac{h}{\alpha}\right)^{1+4\gamma/(\pi-\gamma)} \\ & - \left[\frac{2}{\pi^2}\,G_+^3(3\mathrm{i})\left(\frac{h}{\alpha}\right)^3\ln\frac{h}{\alpha}\right]_{\gamma=\pi/3}\Bigg\} \end{aligned} \tag{B.14}$$

$$\begin{aligned} 2s^z_B(h) = -\mathrm{i}\sqrt{\frac{2}{\pi(\pi-\gamma)}}\Bigg\{ & \gamma a_1\frac{h}{\alpha} + \frac{\pi-\gamma}{2}\,b_1\,\left(\frac{h}{\alpha}\right)^{2\gamma/(\pi-\gamma)} \\ & \left(2\gamma a_{1,2} + \frac{\gamma}{3}\,a_{1,1} + \gamma a_1\frac{G_+(\mathrm{i}3\pi/\gamma)}{G_+(\mathrm{i}\pi/\gamma)}\right)\left(\frac{h}{\alpha}\right)^3 \\ & + \left((\pi-\gamma)a_{1,3} + \frac{\pi+\gamma}{2(\pi-\gamma)}\,\frac{b_1^2 b_{1,2}}{a_1} + \gamma\frac{b_1^3}{a_1}\,\frac{G_+(\mathrm{i}3\pi/g)}{G_+(\mathrm{i}\pi/g)}\right)\left(\frac{h}{\alpha}\right)^{1+4\gamma/(\pi-\gamma)} \\ & + \left(\frac{2\gamma(\pi-\gamma)}{\pi+\gamma}b_{1,3} + \frac{\pi-\gamma}{6}b_{1,1} + \frac{\pi-\gamma}{2}b_{1,3} + \frac{\pi-\gamma}{2}\,\frac{b_1 a_{1,3}}{a_1}\right)\left(\frac{h}{\alpha}\right)^{6\gamma/(\pi-\gamma)} \\ & + \left(\frac{\gamma(3\pi-\gamma)}{2(\pi-\gamma)}b_{1,2} + \frac{2\gamma^2}{\pi-\gamma}\,\frac{b_1 a_{1,2}}{a_1} + \frac{\gamma(\pi+\gamma)}{\pi-\gamma}\frac{G_+(\mathrm{i}3\pi/\gamma)}{G_+(\mathrm{i}\pi/\gamma)}\right)\left(\frac{h}{\alpha}\right)^{2+2\gamma/(\pi-\gamma)} \\ & + \frac{2\gamma(\pi-\gamma)}{\pi+\gamma}\,\frac{b_{1,3}}{a_1}\,\left(\frac{h}{\alpha}\right)^{8\gamma/(\pi-\gamma)-1} \\ & + \pi\left[\frac{c_1}{9}\,\frac{h}{\alpha}\ln\frac{h}{\alpha} + \left(\frac{c_1 c_{1,2}}{3^5 a_1} + \frac{c_{1,2}}{27}\right)\left(\frac{h}{\alpha}\right)^3\ln^2\frac{h}{\alpha}\right. \\ & \left. + \left(\frac{c_1^2}{9a_1}\,\frac{G_+(9\mathrm{i})}{G_+(3\mathrm{i})} + \frac{c_{1,1}}{27\mathrm{i}}\right)\left(\frac{h}{\alpha}\right)^3\ln\frac{h}{\alpha}\right]_{\gamma=\pi/3}\Bigg\} \end{aligned} \tag{B.15}$$

From these expressions, χ can be obtained. Let us consider the special case of free Fermions, i.e., $\gamma = \pi/2$. Eq. (19) implies $\kappa \equiv 0$ so that $G_+ \equiv G_- \equiv 1$. Furthermore, from (27a)-(27d), (B.1)-(B.10), the only non-vanishing coefficients are

$$a_0 = \mathrm{i}\frac{2}{\pi}\,,\; a_1 = \mathrm{i}\frac{4}{\pi}\,,\; a_{0,1} = -\mathrm{i}\frac{2}{\pi}\,,\; a_{1,1} = -\mathrm{i}\frac{4}{\pi},$$

so that

$$\widetilde{g}_+^{(1)}(k) + \widetilde{g}_+^{(2)}(k) = \mathrm{i}\frac{2}{\pi}\left(\frac{1}{k+2\mathrm{i}}\mathrm{e}^{-2B} - \frac{1}{k+6\mathrm{i}}\mathrm{e}^{-6B}\right)\left(1+\frac{1}{N}\right) + \mathrm{o}\left(\mathrm{e}^{-6B}\right).$$

Note that this is the expansion of $\rho_0(x+B)$ in Fourier space. Equations (B.12), (B.13) are equivalent in the free-Fermion case and yield

$$\mathrm{e}^{-2B} = \frac{h}{\alpha}\left(1+\left(\frac{h}{\alpha}\right)\right) + \mathrm{o}\left(h^2\right).$$

Finally, the sum of (B.14), (B.15) can be simplified to

$$\begin{aligned} s^z(h) &= \frac{2}{\pi}\left(\frac{h}{\alpha}+\frac{2}{3}\left(\frac{h}{\alpha}\right)^3\right)\left(1+\frac{1}{N}\right) + \mathrm{o}\left(h^3\right) \\ \chi(h) &= \frac{1}{\pi}\left(1+\frac{1}{2}h^2\right)\left(1+\frac{1}{N}\right) + \mathrm{o}\left(h^2\right), \end{aligned} \tag{B.16}$$

where we have set $\alpha = 2J$ for $\gamma = \pi/2$. Equation (B.16) is in agreement with the exact result (7) within the first two orders.

As far as the isotropic case $\gamma = 0$ is concerned, note that (39), (40) include already next-leading terms for the boundary magnetization and susceptibility. Logarithmic corrections to the finite bulk susceptibility, eq. $(35a)$ with $\gamma = 0$, have been calculated by BA-techniques for PBC [34]:

$$\chi_{\mathrm{bulk}}(h) = \frac{1}{J\pi^2}\left[1+\frac{1}{2\ln(\widetilde{h}_0/h)} - \frac{\ln\ln(\widetilde{h}_0/h)}{4(\ln(\widetilde{h}_0/h))^2}\right] + \mathrm{o}\left(\ln^{-2}(h)\right), \tag{B.17}$$

with $\widetilde{h}_0 = \alpha \mathrm{e}^{-1/8}\pi^{-1/4}$. The scale $\widetilde{h}_0$ has been determined such that no terms $\mathrm{O}\left(\ln^{-2} h\right)$ appear in (B.17).

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